Thermal Hall Conductivity of High Temperature Superconductors: Quantization and Scaling

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(February 1, 2008)

Presented is the theory of thermal Hall conductivity κ_{xy} in the vortex state of high temperature cuprate superconductors in the clean limit. We show that $\lim_{T \to 0} \kappa_{xy}/T$ is a *staircase* function of $1/B$ with an envelope that scales as $1/B$. The relation to the experiments is discussed.

Fifteen years after the discovery of high temperature superconductivity in cuprates [1], the search for the "final" theory continues unabated. Nevertheless, certain important clues about the elements that such a theory must contain appear to be established. One of the most significant results of the past few years is that, in the superconducting state, cuprates seem to be well described by the familiar BCS-type formalism with Cooper pairs binding in the d-wave channel [2]. This is a far from trivial observation in the materials known to exhibit strong correlations. Soon after the original discovery, Anderson [3] identified one of the key features of the new superconductivity: the materials are basically two-dimensional with most of the action relevant for superconductivity taking place in the CuO_2 planes. The reduced dimensionality and the presence of nodal points on an otherwise gapped Fermi surface governs the low temperature properties of the high-T_c superconductors (HTS). Corroborating evidence for the BCS character of the fermionic excitations comes from diverse spectroscopic and transport experiments [4, 5, 6, 7].

Especially informative probe of the quasiparticle dynamics is the thermal Hall conductivity, κ_{xy} [8], particularly since phonons, which usually contribute to the longitudinal thermal conductivity, κ_{xx}, do not contribute to κ_{xy} by the virtue of their being electrically neutral. In addition, from the theoretical point of view, in the leading "nodal" approximation, κ_{xy} vanishes [9, 10, 11] and one must consider curvature terms. For these reasons a special opportunity emerges to scrutinize, both theoretically and experimentally, the extent to which the fermionic quasiparticles in HTS exhibit the BCS-type behavior.

Our starting point is a 2-dimensional Bogoliubov-de Gennes Hamiltonian in the vortex state

$$H_{BdG} = \sigma_3 \frac{\left(\mathbf{p} - \sigma_3 \frac{e}{c} \mathbf{A}\right)^2}{2m^*} - \sigma_3 \mu + \sigma_1 e^{-i\sigma_3 \phi/2} \Delta(\mathbf{p}) e^{-i\sigma_3 \phi/2} \tag{1}$$

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where $\mathbf{A}(\mathbf{x})$ is the vector potential associated with the uniform external magnetic field $\mathbf{B}$, $\mathbf{p}$ is a momentum operator, and σ's are Pauli matrices operating in the Nambu space. The vortex phase fields satisfy $\nabla \times \nabla \phi(\mathbf{x}) = 2\pi \hat{z} \sum_i \delta(\mathbf{x} - \mathbf{x}_i)$ with $\mathbf{x}_i$ denoting the vortex positions and $\delta(\mathbf{x} - \mathbf{x}_i)$ being a 2D Dirac delta function. For a $d_{x^2-y^2}$-wave superconductor $\Delta(\mathbf{p}) = \frac{\Delta_0}{p_F^2}(p_x^2 - p_y^2)$.

Following Franz and Tesanovic [12] (see also [11, 13, 14]), we divide the vortices into two sets A and B, positioned at $\{\mathbf{x}_i^A\}$ and $\{\mathbf{x}_i^B\}$ respectively (see Fig. 1) and define two phase fields $\phi^A(\mathbf{x})$ and $\phi^B(\mathbf{x})$ such that $\nabla \times \nabla \phi^\alpha(\mathbf{x}) = 2\pi \hat{z} \sum_i \delta(\mathbf{x} - \mathbf{x}_i^\alpha)$, $\alpha = A, B$. The Hamiltonian (1) is then transformed into [12]

$$\mathcal{H} = U^\dagger H_{BdG} U = \sigma_3 \frac{(\mathbf{p} - \sigma_3 \mathbf{v} + \mathbf{a})^2}{2m^*} - \sigma_3 \mu + \sigma_1 \Delta(\mathbf{p} + \mathbf{a}) \tag{2}$$

using the unitary operator

$$U = e^{i\chi + i\sigma_3 \Phi} \tag{3}$$

where $\chi = \frac{1}{2}(\phi_A - \phi_B)$ and $\Phi = \frac{1}{2}(\phi_A + \phi_B) = \frac{1}{2}\phi$. In Eq. (2), $\mathbf{v} = \frac{1}{2}\nabla\phi - \frac{e}{c}\mathbf{A}$ is the superfluid velocity and $\mathbf{a} = \frac{1}{2}(\nabla\phi_A - \nabla\phi_B)$ is the Berry gauge field which imposes the condition that a quasiparticle wavepacket encircling an $\frac{hc}{2e}$ vortex must pick up an overall minus sign.

In addition to keeping the wavefunctions single-valued, the advantage of this "bipartite" singular gauge transformation is that for a periodic arrangement of vortices (Abrikosov vortex lattice) the resulting Hamiltonian (2) is itself periodic. This is not true of Hamiltonian (1). Therefore, the eigenstates of (2) can be expressed through the familiar Bloch waves $\psi_{n\mathbf{k}}(\mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x}} u_{n\mathbf{k}}(\mathbf{x})$ labeled by one discrete quantum number, the band index n, and two continuous quantum numbers, the vortex crystal momenta k_x, k_y that range in the first Brillouin zone. Note that $u_{n\mathbf{k}}(\mathbf{x})$ is not periodic with the periodicity of the vortex lattice, but with the periodicity of the vortex sublattice containing a unit of *electronic* flux $\frac{hc}{e}$ (see Fig. 1).

By extracting the plane wave part of the Bloch states

FIG. 1: Example of A and B sublattices for the square vortex arrangement.

FIG. 2: Scaling of the field induced quasiparticle gap Δ_m (open circles) with the magnetic field and the chemical potential μ (measured from the bottom of the tight-binding band). The quantized values of the σ_{xy}^{spin} are also shown (solid line). Magnetic length, l, is in units of the tight-binding lattice constant a and energies are in units of the hoping energy t; the results are for a square vortex lattice with $\Delta_0 = 0.1t$. The dashed line is the envelope scaling function.

we can define a Hamiltonian

$$\mathcal{H}(\mathbf{k}) = \sigma_3 \frac{(\mathbf{p} + \mathbf{k} - \sigma_3\mathbf{v} + \mathbf{a})^2}{2m^*} - \sigma_3\mu + \sigma_1\Delta(\mathbf{p} + \mathbf{k} + \mathbf{a}) \tag{4}$$

where $\mathcal{H}(\mathbf{k}) = e^{-i\mathbf{k}\cdot\mathbf{x}}\mathcal{H}e^{i\mathbf{k}\cdot\mathbf{x}}$. We now wish to point out an important feature of $\mathcal{H}(\mathbf{k})$ in the case when the vortex lattice has an inversion symmetry. As shown in Ref.[14] an operator $\mathcal{P} = i\sigma_2\mathcal{C}\mathcal{I}$, where $\mathcal{C}$ represents charge conjugation and $\mathcal{I}$ takes $\mathbf{x}$ into $-\mathbf{x}$, with the following property

$$\mathcal{P}^{-1}\mathcal{H}(\mathbf{k})\mathcal{P} = -\mathcal{H}(\mathbf{k}); \quad \langle u_{n\mathbf{k}}|\mathcal{P}|u_{n\mathbf{k}}\rangle = 0. \tag{5}$$

This means that for every energy band $\epsilon_{n\mathbf{k}}$ there is another $\epsilon_{m\mathbf{k}}$ such that $\epsilon_{n\mathbf{k}} = -\epsilon_{m\mathbf{k}}$, i.e. the band spectrum has reflection symmetry about the Fermi level and if a band were to cross the Fermi level ($\epsilon_{n\mathbf{q}} = 0$ for some $\mathbf{q}$) then there would have to be a twofold degeneracy at $\mathbf{q}$. However, by the von Neumann-Wigner "non-crossing" theorem [15], the degeneracy unrelated to symmetry cannot happen for a time reversal breaking Hamiltonian which depends only on two continuous parameters. Thus, the quasiparticle spectrum of the $d_{x^2-y^2}$ superconductor in the vortex state is gapped by a (direct) gap $\Delta_m \ll \Delta_0$ unless a third parameter is fine tuned, e.g. the band crossing at the Fermi level can be achieved by fine-tuning the chemical potential μ.

If we rescale all coordinates by the magnetic length $l = \sqrt{c/eB}$ (see Fig. 1), $\mathbf{x} \to l\mathbf{x}$, then

$$\mathcal{H}(\mathbf{k}, l, \mu, \Delta_0) \to \frac{1}{l^2}f(l\mathbf{k}, l^2\mu, \frac{\Delta_0}{p_F^2}), \tag{6}$$

where f is a universal (operator) function. Consequently, the small band gap Δ_m at the Fermi level, which is equal to the minimum of the lowest positive eigen-energy of $\mathcal{H}(\mathbf{k}, l, \mu)$ with respect to $\mathbf{k}$, is also a universal function that can be written as

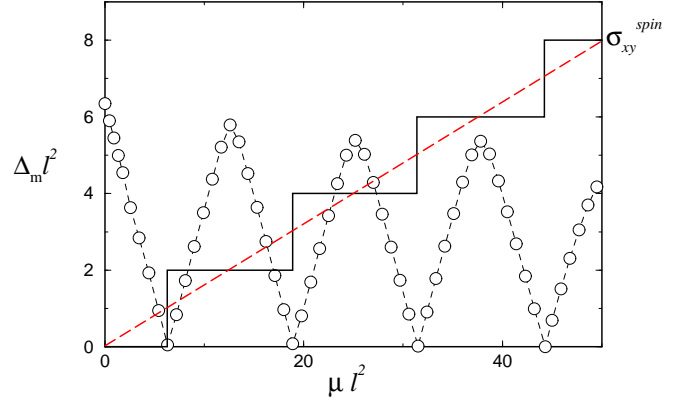$$\Delta_m(B, \mu, \Delta_0) = B \times F\left(\frac{\mu}{B}, \frac{\Delta_0}{p_F^2}\right). \tag{7}$$

Thus, in order to determine the dependence of Δ_m on the magnetic field B, all we need to know is the dependence of Δ_m on μ for some fixed B and $\frac{\Delta_0}{p_F^2}$, and then use the scaling relation (7). This dependence is determined numerically by diagonalizing a tight-binding version [14] of the Hamiltonian (4) close to the bottom of the tight-binding band where we expect to recover the continuum theory (4). The numerical calculations confirm the scaling (7) which gives us confidence in relating the continuum results to the tight-binding approximation. As shown in Fig. 2, for a fixed value of $\frac{t}{\Delta_0} = \alpha_D = 10$, where t is the tight-binding hopping constant, $\frac{1}{B}\Delta_m(\frac{\mu}{B})$ is a saw-tooth function with a period of approximately 4π.

In Ref. [14] it was demonstrated that the gapped quasiparticle spectrum leads to the quantization of the spin Hall conductivity σ_{xy}^{spin} (see also Ref. [11]), which is in turn related to the thermal Hall conductivity, κ_{xy}, via the Wiedemann-Franz law

$$\lim_{T\to 0} \frac{\kappa_{xy}}{T} = \frac{4\pi^2}{3}\left(\frac{k_B}{\hbar}\right)^2 \sigma_{xy}^{spin}(B). \tag{8}$$

Because the quantization of σ_{xy}^{spin} is topological in origin [14], any continuous change in a parameter of the Hamiltonian results in the same quantized value of σ_{xy}^{spin} unless the quasiparticle gap collapses. Therefore, for a fixed Dirac anisotropy α_D, by virtue of Eq. (6), the dependence of σ_{xy}^{spin} on B and μ can be expressed entirely as a dependence of σ_{xy}^{spin} on $\frac{1}{B}\Delta_m(B, \mu)$, i.e.

$$\sigma_{xy}^{spin}(B, \mu) = G\left(\frac{\mu}{B}\right), \tag{9}$$

where G is a universal function of its argument that in addition depends on the geometry of the vortex lattice.
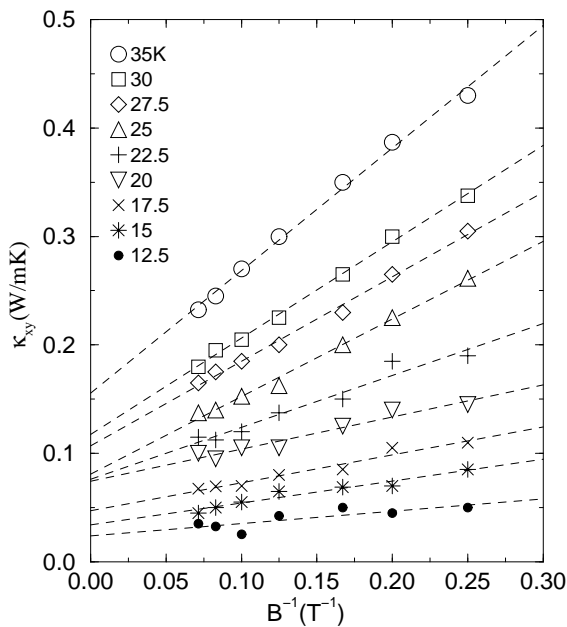
FIG. 3: Thermal Hall conductivity data of Zhang et. al. [8] for $B > 4T$ plotted vs. B^{-1}.

For a fixed (large) value of B the numerical computation of σ_{xy}^{spin} can be readily accomplished. The results for a square vortex lattice and $\alpha_D = 10$ are displayed in Fig. 2 where it is seen that σ_{xy}^{spin} is a stair-case function of $\frac{\mu}{B}$ which starts at zero at empty filling and then jumps by a multiple of $2\frac{\hbar}{8\pi}$. The band crossings, which are responsible for the changes in σ_{xy}^{spin}, occur at symmetry points in the Brillouin zone, and by the symmetry of the square vortex lattice, the steps are bound to come in even integers [16].

Thus we arrive at the main result of this Letter shown in Fig. 2: the envelope of the $\sigma_{xy}^{spin}(B)$ scales as B^{-1} and by Eq. (8)

$$\lim_{T \to 0} \left(\frac{\kappa_{xy}}{T} \right) \propto \frac{1}{B} \qquad (10)$$

This expression is reminiscent of the electrical Hall conductivity in the 2D electron gas.

Recently, measurements of κ_{xy} were conducted by Ong's group [8] on YBCO samples with a very long mean free path. These experiments were carried out over a wide range of magnetic fields (up to $\sim 14T$) and at temperatures from $T \sim 12.5K$ to above the superconducting transition $T_c \sim 90K$. Unfortunately, the experiments are resolution limited below $12.5K$ as signal becomes too weak. In Fig. 3 we re-analyze the data of Ref. [8]. It is seen that for the magnetic fields above $4T$, $\kappa_{xy} \propto C + B^{-1}$ which is, apart from the finite intercept, in agreement with our theory. At fields $B < 4T$, κ_{xy} decreases with decreasing B and vanishes at $B = 0$ [8]. At low magnetic fields $\frac{1}{B}$ divergence of κ_{xy} is cut-off by disorder

i.e. $\kappa_{xy} = \frac{\rho_{xy}}{\rho_{xx}^2 + \rho_{xy}^2}$ with non-vanishing longitudinal quasiparticle thermal resistivity ρ_{xx}. Even in the presence of weak disorder, we still expect $\rho_{xy} \propto B$ and ρ_{xx} to be approximately field independent. Therefore, the transverse thermal conductivity in the presence of disorder should vanish in the limit of vanishing B. We must admit that the origin of the residual thermal conductivity at $\frac{1}{B} = 0$, evident in Fig. 3, remains mysterious to us and we can only speculate that it is not of quasiparticle origin.

In summary, based on a general analysis of the full *non-linearized* Bogoliubov-de Gennes equations, we argued that magnetic field B will induce a small gap Δ_m in the quasiparticle spectrum which is a non-monotonic function of the magnetic field. Rather, Δ_m vanishes at some special values of μ/B which depend on the details of the vortex lattice and the Dirac cone anisotropy (Fig. 2). The dependence of κ_{xy} on B is entirely due to this non-monotonic behavior of Δ_m, since κ_{xy}/T is a topological quantity and therefore can change only at the band crossings [14]. The topological quantization of κ_{xy} was also discussed in the Ref. [11]. However, we wish to point out a significant qualitative difference between the results presented here and those of Ref. [11]: as we argued before κ_{xy} is a quantized staircase function of $1/B$ with an *envelope* that itself scales as $1/B$, while Ref. [11] states that κ_{xy}/T can take on only one of the three allowed values $0, \pm2$ and is otherwise field-independent. Consequently, in a typical experimental situation, the explicit values for κ_{xy} obtained from these two works will differ significantly. Still, there is an agreement on the fact that since the quasiparticle spectrum is gapped κ_{xy} does not obey simple Simon-Lee scaling, at least when the temperature is comparable to the quasiparticle gap.

[1] J. G. Bednorz and K. A. Muller, Z. Phys. **64** 188 (1986).
[2] D. J. Van Harlingen, Rev. Mod. Phys. **67**, 515 (1995).
[3] P. W. Anderson, Science **235**, 1196 (1987).
[4] M. B. Walker and M. F. Smith, Phys. Rev. B **61**, 11285 (2000).
[5] H. Ding *et. al.*, Phys. Rev. B **54**, R9678 (1996).
[6] M. Chiao *et. al.*, cond-mat/9910367.
[7] J. Orenstein and A. J. Millis, Science **288**, 468 (2000).
[8] Y. Zhang *et. al.* Phys. Rev. Lett. **86**, 890 (2001).
[9] S. H. Simon and P. A. Lee, Phys. Rev. Lett. **78**, 1548 (1997).
[10] J. Ye, Phys. Rev. Lett. **86**, 316 (2001).
[11] A. Vishwanath, Phys. Rev. Lett. **87**, 217004 (2001); A. Vishwanath cond-mat/0104213.
[12] M. Franz and Z. Tešanović, Phys. Rev. Lett. **84**, 554 (2000); O. Vafek, A. Melikyan, M. Franz, Z. Tešanović, Phys. Rev. B **63**, 134509 (2001).
[13] L. Marinelli, B. I. Halperin and S. H. Simon, Phys. Rev. B **62** 3488 (2000).

[14] O. Vafek, A. Melikyan, and Z. Tešanović, Phys. Rev. B **64**, 224508 (2001) and references therein.

[15] J. von Neumann and E. Wigner, *Physik. Z.*, **30** 467 (1927).

[16] The trivial double degeneracy of each band due to spin is ignored in this calculation.